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# Calculated electronic structure and measured X-ray photoemission spectrum of $UAuSb_2$

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**Abstract**

The electronic band structure for the tetragonal ferromagnetic compound $UAuSb_2$ was calculated by the full potential LMTO method. The XPS was measured on single crystals freshly cleaved under high vacuum. The calculated spectrum for the valence band compares well with the measured one. The calculated magnetic moment is significantly smaller than estimated from measurements of magnetization. The cylindrical shape of the Fermi surface is an indication of quasi-two dimensionality of the properties of $UAuSb_2$ related to its crystal structure having the unit cell elongated along the tetrahedral direction.


*Keywords:* Actinide alloys and compounds; Electronic band structure; Photoelectron spectroscopies

## 1. Introduction

The uranium-transition metal diantimonides $UTSb_2$ (T = transition metal) belong to a numerous family of ternary compounds crystallizing in a tetragonal structure of the $HfCuSi_2$-type (space group P4/nmm), which can be described as a filled $USb_2$ structure [1]. Due to the layered character of this structure, this kind of compounds can lead to the formation of the quasi-two-dimensional (QTD) electronic states. For example, the dHvA experiments performed for the parent $USb_2$ compound indicate that the QTD electronic state develops in the form of four kinds of nearly cylindrical Fermi surfaces [2] although the c/a ratio of the $USb_2$ unit cell is smaller than that expected for a given $UTSb_2$ representative. The quasi-two dimensionality is closely related to the magnetic unit cell and/or to the unique crystal structure elongated along the tetragonal [0 0 1] direction, which bring about a flat Brillouin zone and produce cylindrical highly corrugated Fermi surface along [0 0 1]. The enhanced cyclotron masses for $USb_2$ found in this experiment correspond well to an experimental value of the electronic coefficient of specific heat $\gamma$ (25 mJ/(K$^2$ mol)).

The first studies of $UTSb_2$ series have been performed on the polycrystalline samples [3] and very recently some of these ternaries with T = Co [4,5], Ni [6,7] and Cu [8] on single-crystalline samples. Most of $UTSb_2$ compounds have been found to order magnetically at low temperatures and characterized as semimetallic Kondo lattices with strongly screened uranium magnetic moments [3–8]. They have first of all revealed a strong competition of the crystal field effects with the Kondo-like and magnetic order interactions. For example the resistivity and magnetoresistance data taken for the Co-containing compound were interpreted in terms of the two-dimensional weak localization (2DWL) effect [5]. The electron effective mass at 2 K was established to be about 70 $m_0$, which is quite large in case of a ferromagnetic system. All these give rise to interesting features in studies of their anomalous behavior at low temperatures.

In the framework of our systematic investigation of this group of ternaries we have recently extended our interest to $UAuSb_2$. Some preliminary magnetic study of this compound have shown two magnetic transitions, a ferromagnetic one at $T_C = 31$ K and probably an antiferromagnetic one at 43 K [9]. In this paper

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Table 1
Coordinates of atomic positions in units of lattice parameters ($a = 4.3750$ Å for $x$, $y$; $c = 9.831$ Å for $z$) and radii of overlapping ($S_{asa}$) and non-overlapping ($S_{mt}$) muffin-tin spheres, in atomic units

| Atom | Site type | $x$ | $y$ | $z$ | $S_{asa}$ | $S_{mt}$ |
|---|---|---|---|---|---|---|
| U | 2c | 1/4 | 1/4 | 0.2438 | 3.701 | 3.186 |
| Au | 2b | 3/4 | 1/4 | 1/2 | 3.005 | 2.587 |
| Sb | 2c | 1/4 | 1/4 | 0.6862 | 3.255 | 2.802 |
| Sb | 2a | 3/4 | 1/4 | 0 | 3.396 | 2.923 |

we report the results of electronic band structure calculations and photoemission examinations of single crystalline samples of $UAuSb_2$ [9].

## 2. Calculations of the electronic structure

Calculations of the electronic structure were performed by the LMTO method using the LmtART code (version 6.50) [10,11] both in the atomic spheres approximation (ASA) and for full potential (FP). Results of the latter, as the more accurate method, will be reported below in details. The differences between these two approaches in practice appear to be minor, as in particular for the calculated X-ray photoemission spectrum (XPS) which is in the focus of present paper. The exchange-correlation potential in the form proposed by Vosko–Wilk–Nussair [12] was used together with gradient corrections according to Perdew et al. [13]. Calculations were done in semirelativistic approximation with the spin–orbit coupling, and for spin-polarized case.

The compound $UAuSb_2$ crystallizes in a tetragonal structure belonging to the space group P4/nmm, with two formula units in the unit cell. The relevant crystallographic data are collected in Table 1 taken from Ref. [9]. The following experimental lattice parameters: $a = 4.375$ Å, $c = 9.831$ Å, determined at room temperature were taken for computations. In the calculations scheme 12 electrons of U ($5f^3 6p^6 6d^1 7s^2$) were treated as valence electrons and 2 ($6s^2$) as semicore ones. For Au there are 11 valence electrons ($5d^{10} 6s^1$) and for Sb (in both crystallographic inequivalent positions), five valence ($5s^2 5p^3$) and 10 semicore electrons ($4d^{10}$). The total energy self-consistency up to 0.01 mRy, the charge-density self-consistency $1 \times 10^{-4}$ e, the magnetization self-consistency $2 \times 10^{-4}\ \mu_B$ were attained at the end of iterations. The number of $k$-points in the Brillouin zone was 1728. The atomic radii for overlapping spheres ($S_{asa}$) and for non-overlapping muffin-tin spheres ($S_{mt}$) are specified in the columns 6th and 7th of Table 1, respectively. The electron density in the region between non-overlapping spheres was expanded into 31,750 plane waves.

## 3. Results of calculations

Results of the calculations of the electronic structure are summarized as the density of states (DOS) plots in Figs. 1 and 2.

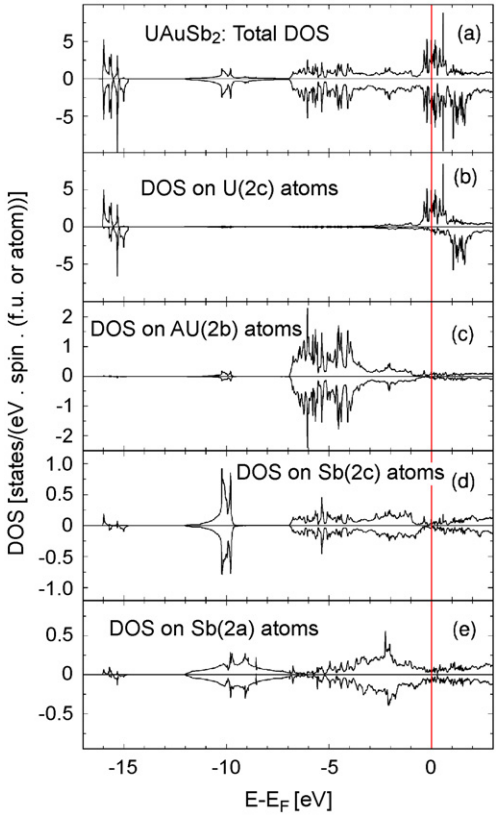


Fig. 1. Calculated total DOS (a) and site contributions from the U, Au and Sb atoms (in the case of the latter atom there are two positions in the (2c) and (2a) sites) are presented in panels (b)–(e), respectively.

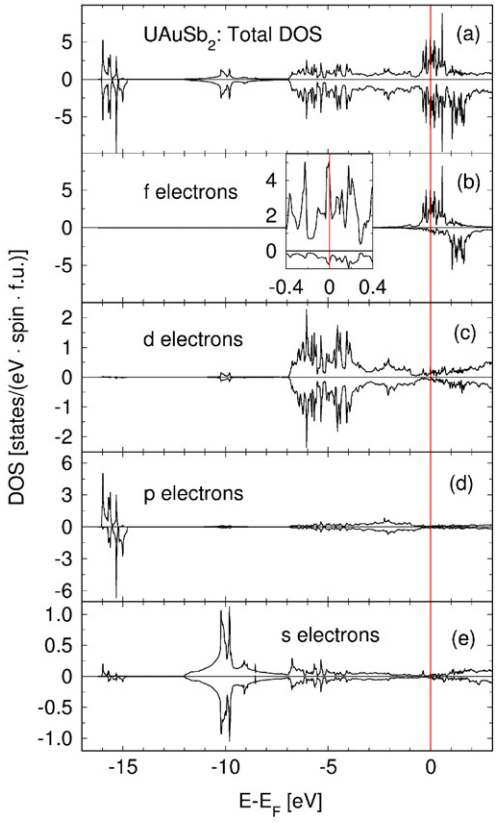


Fig. 2. Partial DOS from the f, d, p and s electrons in panels (b)–(e) with total DOS, (a) for comparison. Inset in the panel (b) presents extended energy scale around the Fermi energy.